

Matrix Algebras in Non-Hermitian Quantum Mechanics

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Abstract

In principle, non-Hermitian quantum equations of motion can be formulated using as a starting point either the Heisenberg's or the Schrödinger's picture of quantum dynamics. Here it is shown in both cases how to map the algebra of commutators, defining the time evolution in terms of a non-Hermitian Hamiltonian, onto a non-Hamiltonian algebra with a Hermitian Hamiltonian. The logic behind such a derivation is reversible, so that any Hermitian Hamiltonian can be used in the formulation of non-Hermitian dynamics through a suitable algebra of generalized (non-Hamiltonian) commutators. These results provide a general structure (a template) for non-Hermitian equations of motion to be used in the computer simulation of open quantum systems dynamics.

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It can be said that the recent experimental realizations of \mathcal{PT} -symmetric time evolution by means of optical waveguides [1, 2] has renewed the interest in non-Hermitian quantum mechanics [3]. Besides practical applications to such recent developments [1, 2], non-Hermitian theories are interesting since they can be thought of as tools for computational modelling of open quantum systems dynamics [4]. It is known, in fact, that open quantum system dynamics can be represented in terms of non-Hermitian quantum trajectory segments interspersed by quantum transitions [4]. It is also worth mentioning that an analysis of the classical limit of non-Hermitian quantum dynamics [5] has revealed geometrical structures of phase space that are represented in terms of dissipative brackets [6]. Such brackets were originally proposed by Grmela [6] and later widely discussed by Ottinger, in his approach to beyond equilibrium thermodynamics [7]. Moreover, Ottinger himself has very recently provided an approach to the quantization of such a dissipative dynamics [8] by means of non-Hermitian quantum trajectories and jumps [4], hence providing some kind of logical *short-circuit* to the quantum trajectory representation of open quantum system dynamics [4]. Despite such interesting issues, so far attempts to characterize the general features of non-Hermitian quantum dynamics have been few in number. A very interesting exception is the recent work of Graefe and Schubert [9], where preliminary steps of such an analysis are performed within a coherent-state representation.

In this brief communication, the focus is not on specific applications but on the derivation of a general structure (a template) for non-Hermitian equations of motion. In full generality, quantum commutators defined in terms of a non-Hermitian Hamiltonian are mapped onto non-Hamiltonian commutators [10–12] defined in terms of the Hermitian part of the Hamiltonian. Since commutators with the Hamiltonian naturally defines dynamics in the Heisenberg picture, such a mapping allows one to immediately identify very general characteristics of non-Hermitian evolution in time. This provides a conceptual connection between non-Hermitian and non-Hamiltonian (or almost-Lie) dynamics. In particular, the logic behind the mapping is reversible so that any Hermitian Hamiltonian can be used in the formulation of non-Hermitian dynamics by means of a suitable algebra of generalized (non-Hamiltonian) commutators. It is not difficult to foresee that this can be exploited for devising novel algorithms to simulate open quantum systems. In fact, it is known that open quantum systems can be studied by evolving the conserved Hamiltonian of the total

system [13] and then measuring properties of the relevant subsystem only. Analogously, one would have to follow the non-Hermitian evolution of the conserved Hamiltonian of the total system and then calculate properties of just a relevant part. The use of non-Hermitian evolution (in place of the natural Hamiltonian dynamics) can provide the computational advantage of reducing the number of degrees of freedom constituting the bath of the relevant quantum subsystem [14]. Such a logic is very well-known in the field of classical molecular dynamics where one can use the non-Hamiltonian evolution of a total conserved Hamiltonian in order to impose thermodynamic constraints onto a relevant subsystem [15–17].

Let us consider a non-Hermitian Hamiltonian operator $\hat{H} \neq \hat{H}^\dagger$ determining the time evolution of an arbitrary quantum observable $\hat{\chi}$ in terms of the commutator

$$i\hbar \frac{d}{dt} \hat{\chi} = [\hat{\chi}, \hat{H}] = \begin{bmatrix} \hat{\chi} & \hat{H} \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \hat{\chi} \\ \hat{H} \end{bmatrix}. \quad (1)$$

Equation (1) displays the matrix structure of the commutator, which was exploited in [10]. For future convenience, a more compact notation can be introduced. To this end, defining the symplectic matrix

$$\mathbf{\Omega} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad (2)$$

and the column vector

$$\mathbf{\chi}_{\hat{H}} = \begin{bmatrix} \hat{\chi} \\ \hat{H} \end{bmatrix}, \quad (3)$$

Eq. (1) can be written as

$$i\hbar \frac{d}{dt} \hat{\chi} = \mathbf{\chi}_{\hat{H}}^\top \cdot \mathbf{\Omega} \cdot \mathbf{\chi}_{\hat{H}} \quad (4)$$

$$= [\hat{\chi}(t), \hat{H}]_{\mathbf{\Omega}}. \quad (5)$$

Equation (4) simply makes apparent the antisymmetric matrix structure of quantum evolution. Such a structure underlies various non-Hamiltonian and non-linear approximations of quantum dynamics [10–12]. Equation (5) simply shows that the matrix structure is equivalent to the commutator, defining a Lie bracket and a Lie algebra of operators in quantum mechanics. The commutator is written putting the matrix $\mathbf{\Omega}$ into evidence. This brings forward the idea [10–12] that more general algebras and brackets can be defined simply by tampering with the definition of $\mathbf{\Omega}$.

The generic non-Hermitian Hamiltonian can always be split in terms of an Hermitian (\hat{H}_+) and an anti-Hermitian part (\hat{H}_-):

$$\hat{H} = \hat{H}_+ + \hat{H}_- , \quad (6)$$

where $\hat{H}_+ = (1/2) (\hat{H} + \hat{H}^\dagger)$ and $\hat{H}_- = (1/2) (\hat{H} - \hat{H}^\dagger)$. In terms of such a decomposition, the commutator with the Hamiltonian also splits into two parts: $[\hat{\chi}, \hat{H}] = [\hat{\chi}, \hat{H}_+] + [\hat{\chi}, \hat{H}_-]$. It is now a matter of simple algebra to show that the commutator of an operator with the non-Hermitian Hamiltonian is equivalent to a non-Hamiltonian commutator of the same observable with only the Hermitian part of the Hamiltonian. To this end, defining the antisymmetric matrix operator

$$\boldsymbol{\Omega}_{-+} \equiv \begin{bmatrix} 0 & 1 + \hat{H}_- (\hat{H}_+)^{-1} \\ -1 - (\hat{H}_+)^{-1} \hat{H}_- & 0 \end{bmatrix} , \quad (7)$$

one finds

$$[\hat{\chi}, \hat{H}]_{\boldsymbol{\Omega}} \equiv \boldsymbol{\chi}_{\hat{H}_+}^T \cdot \boldsymbol{\Omega}_{-+} \cdot \boldsymbol{\chi}_{\hat{H}_+} \quad (8)$$

$$= [\hat{\chi}(t), \hat{H}_+]_{\boldsymbol{\Omega}_{-+}} , \quad (9)$$

where in Eq. (8), following an analogy with Eq. (3), the column vector

$$\boldsymbol{\chi}_{\hat{H}_+} = \begin{bmatrix} \hat{\chi} \\ \hat{H}_+ \end{bmatrix} \quad (10)$$

has been defined. Equation (9) introduces a more general (non-Hamiltonian) commutator than the usual one based on the symplectic matrix. Equations (8) and (9) realize a mapping between a standard commutator in terms of a non-Hermitian Hamiltonian \hat{H} and a non-Hamiltonian commutator defined in terms of \hat{H}_+ , the Hermitian part of \hat{H} .

At this stage, it is worth discussing the starting point of the derivation leading to the non-Hermitian matrix algebra defined by Eqs. (8) and (9). Such a starting point is given by Eq. (1). This amounts to give a more fundamental role to the Heisenberg law of evolution for observables, so that Eqs. (8) and (9) defines an Heisenberg-based non-Hermitian quantum dynamics. Such a choice has some advantages. One of these is that the Dirac's quantum-classical correspondence between commutators and Poisson brackets remains unaltered [18].

It must be remarked that, in order to formulate non-Hermitian dynamics, other authors have decided to give a more fundamental role to the Schrödinger's picture, for example

see [9], and start from non-Hermitian equations of motion for state vectors:

$$\begin{cases} |\dot{\Psi}\rangle = -\frac{i}{\hbar}\hat{H}_+|\Psi\rangle + \frac{\hat{\Gamma}}{\hbar}|\Psi\rangle \\ \langle\dot{\Psi}| = \frac{i}{\hbar}\langle\Psi|\hat{H}_+ + \langle\Psi|\frac{\hat{\Gamma}}{\hbar} \end{cases}, \quad (11)$$

where the Hermitian operator $\hat{\Gamma} = -i\hat{H}_-$ has been introduced. These equations lead to an equation of motion for the density matrix where an anticommutator, $[\dots, \dots]_+$, appears:

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}[\hat{H}_+, \hat{\rho}(t)] + \frac{1}{\hbar}[\hat{\Gamma}, \hat{\rho}(t)]_+. \quad (12)$$

One can note that the equivalence between the Heisenberg and the Schrödinger picture of dynamical evolution is lost when the Hamiltonian is non Hermitian. At this point, it should not be surprising that Eq. (12) can also be put in matrix form. To this end, we can define the general matrix operator (which is neither Hermitian nor antisymmetric)

$$\mathbf{\Lambda} = \begin{bmatrix} 0 & 1 + i\hat{\Gamma}(\hat{H}_+)^{-1} \\ -1 + i(\hat{H}_+)^{-1}\hat{\Gamma} & 0 \end{bmatrix}. \quad (13)$$

Hence, Equation (12) can be rewritten as

$$-i\hbar\frac{d}{dt}\hat{\rho}(t) = \boldsymbol{\rho}_{\hat{H}_+}^T \cdot \mathbf{\Lambda} \cdot \boldsymbol{\rho}_{\hat{H}_+} \quad (14)$$

$$= [\hat{\rho}(t), \hat{H}_+]_{\mathbf{\Lambda}}. \quad (15)$$

Equation (15) introduces a bracket that has an antisymmetric and a symmetric part and, hence, seems to directly implement the original ideas of Grmela [6] within a quantum framework. More in general, Equations (12), (14), and (15) make an immediate contact with theories of dissipation ([6, 7]) and lead to interesting structures of phase space in the classical limit [5, 9].

What is interesting for open quantum system dynamics is that the logic leading to Eq. (8) can be reversed. Consider an Hermitian Hamiltonian operator $\mathcal{H} = \mathcal{H}^\dagger$, having by definition a spectrum of real eigenvalues. Consider also a non-Hermitian operator $\hat{\xi} \neq \hat{\xi}^\dagger$. Upon defining an antisymmetric (but non-Hermitian) matrix $\mathbf{\Omega}_\xi$ as

$$\mathbf{\Omega}_\xi = \begin{bmatrix} 0 & \hat{\xi} \\ -\hat{\xi}^T & 0 \end{bmatrix}, \quad (16)$$

one can define non-Hermitian evolution for any observable in terms of a non-Hamiltonian commutator:

$$i\hbar\frac{d}{dt}\chi = \chi_{\hat{\mathcal{H}}}^T \cdot \mathbf{\Omega}_\xi \cdot \chi_{\hat{\mathcal{H}}} \quad (17)$$

$$= [\hat{\chi}(t), \hat{\mathcal{H}}]_{\Omega_\xi}, \quad (18)$$

where the two-dimensional columns vector

$$\chi_{\hat{\mathcal{H}}} \equiv \begin{bmatrix} \hat{\chi} \\ \hat{\mathcal{H}} \end{bmatrix} \quad (19)$$

has been introduced in analogy with Eqs. (3) and (10). Equations (17) and (18) can be seen as a general way to define non-Hermitian dynamics for arbitrary Hamiltonian $\hat{\mathcal{H}}$ that (at time $t = 0$) have a real spectrum of eigenvalues. It can be argued that the non-Hermitian time evolution introduced by the non-Hamiltonian commutator in the right hand side of Eq. (17) simulates the dynamics of an open quantum systems. Such an inversion of logic can also be applied to the Schrödinger-based non-Hermitian dynamics. Accordingly, Eqs. (14) and (15), together with the definition of the matrix operator (13), can be reinterpreted as defining a non-Hermitian algebra for an arbitrary Hamiltonian operator with real eigenvalues at $t = 0$.

In this brief communication, we have discussed the form taken by the equations of motion in non-Hermitian quantum mechanics in both the Heisenberg's and the Schrödinger's picture. In both cases, one can introduce a suitable algebra of non-Hamiltonian commutators by exploiting the matrix structure of the equations of motion for quantum operators. Inverting the logic, such algebras may be exploited for defining the non-Hermitian evolution in terms of Hamiltonians having a real spectrum of eigenvalues at the initial time. The Heisenberg-based non-Hermitian dynamics preserves Dirac's quantum-classical correspondence between commutators and Poisson brackets [18]. Moreover, already well-developed and tested numerical algorithms for quantum dynamics [19, 20] promise to be more readily applied to such a formulation of non-Hermitian dynamics. At the moment of writing, the classical limit of the Heisenberg-based non-Hermitian quantum dynamics remains to be investigated. In particular, it is to be assessed whether the phase space structure, found by Graefe [5] and Schubert [9] within the Schrödinger-based dynamics, also emerge from Heisenberg-based non-Hermitian quantum mechanics.

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